



## wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 05:01 pm GMT

PDB ID : 4ADV  
EMDB ID : EMD-2017  
Title : Structure of the E. coli methyltransferase KsgA bound to the E. coli 30S ribosomal subunit  
Authors : Boehringer, D.; O'Farrell, H.C.; Rife, J.P.; Ban, N.  
Deposited on : 2012-01-03  
Resolution : 13.50 Å (reported)  
Based on initial models : 2AVY, 1QYR

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

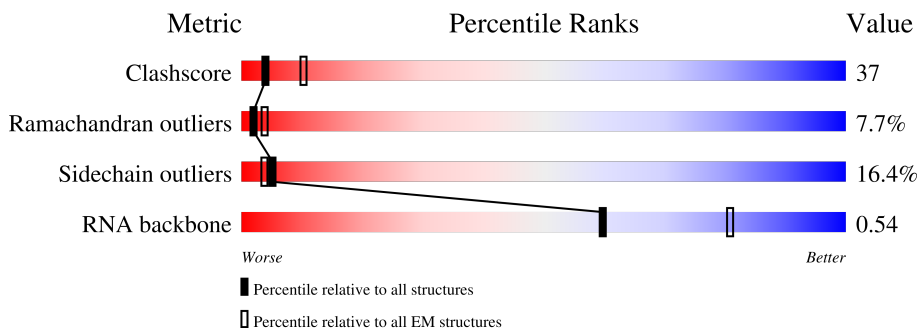
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 13.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1542	6% (Poor fit) 23% (0 outliers), 55% (1 outlier), 13% (2 outliers), 9% (3+ outliers)
2	B	240	45% (Poor fit) 19% (0 outliers), 52% (1 outlier), 19% (2 outliers), 9% (3+ outliers)
3	C	232	76% (Poor fit) 27% (0 outliers), 48% (1 outlier), 13% (2 outliers), 11% (3+ outliers)
4	D	205	27% (Poor fit) 27% (0 outliers), 53% (1 outlier), 19% (2 outliers)
5	E	166	48% (Poor fit) 28% (0 outliers), 50% (1 outlier), 11% (2 outliers), 10% (3+ outliers)
6	F	135	13% (Poor fit) 24% (0 outliers), 37% (1 outlier), 11% (2 outliers), 26% (3+ outliers)
7	G	178	42% (Poor fit) 26% (0 outliers), 46% (1 outlier), 11% (2 outliers), 16% (3+ outliers)

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Mol	Chain	Length	Quality of chain
8	H	129	
9	I	129	
10	J	103	
11	K	128	
12	L	123	
13	M	117	
14	N	100	
15	O	89	
16	P	82	
17	Q	83	
18	R	74	
19	S	91	
20	T	86	
21	U	71	
22	V	252	

## 2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 50888 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1410	30262	13496	5559	9797	1410	0	0

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	218	1704	1081	305	311	7	0	0

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	206	1624	1028	305	288	3	0	0

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	205	1643	1026	315	298	4	0	0

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	150	1105	687	211	201	6	0	0

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	100	817	515	148	148	6	0	0

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	150	1174	730	226	214	4	0	0

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	129	979	616	173	184	6	0	0

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	127	1022	634	206	179	3	0	0

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	98	786	493	150	142	1	0	0

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	117	877	540	174	160	3	0	0

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	123	955	590	196	165	4	0	0

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	114	883	546	178	156	3	0	0

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	88	Total	C	N	O	S	0	0
			716	440	146	129	1		

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	U	51	425	265	86	73	1	0	0

- Molecule 22 is a protein called RIBOSOMAL RNA SMALL SUBUNIT METHYLTRANSFERASE A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	V	252	1949	1241	336	359	13	0	0

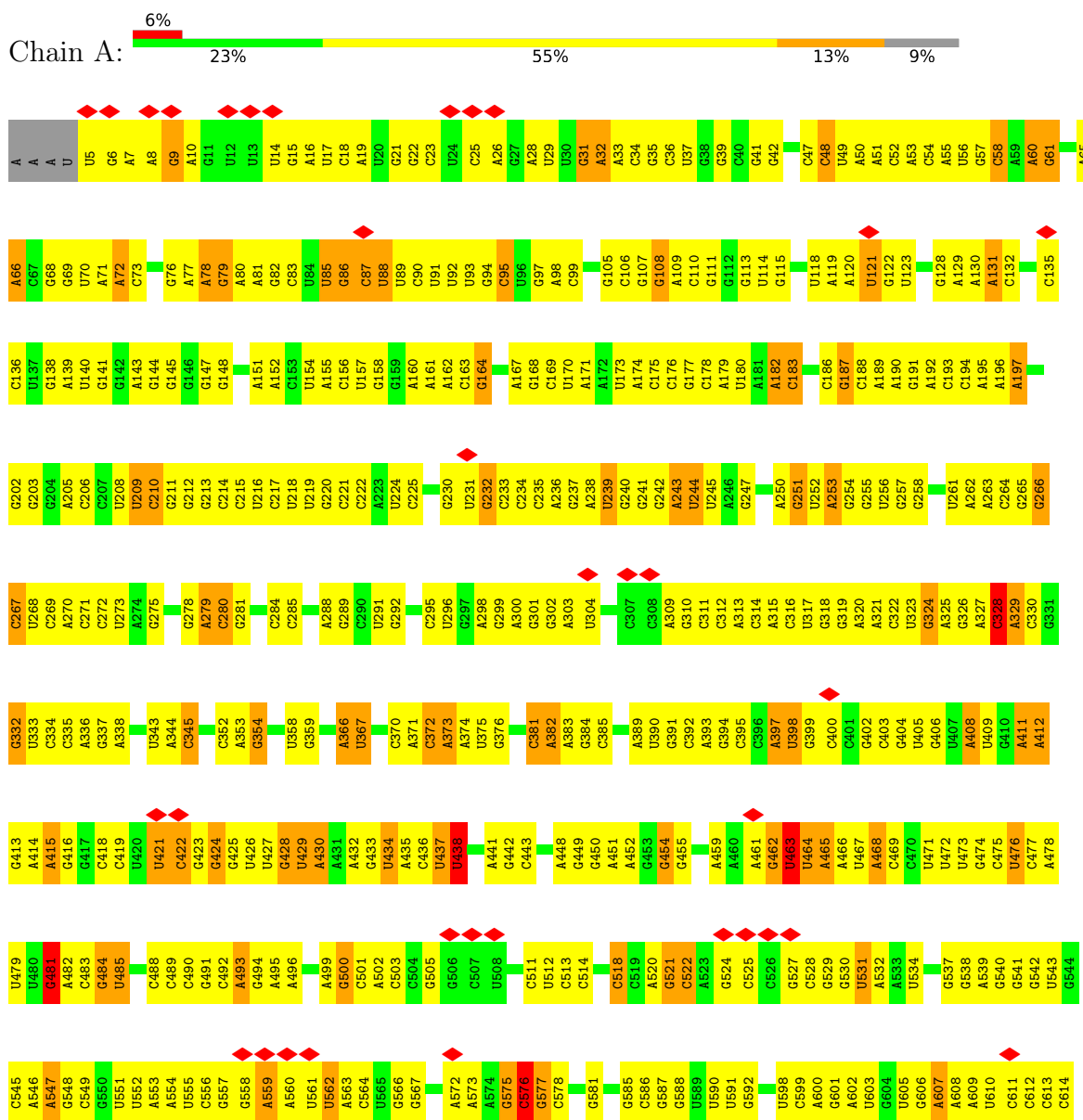
- Molecule 23 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
23	V	139	139	139	0

### 3 Residue-property plots [i](#)

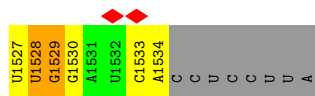
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: 16S RIBOSOMAL RNA

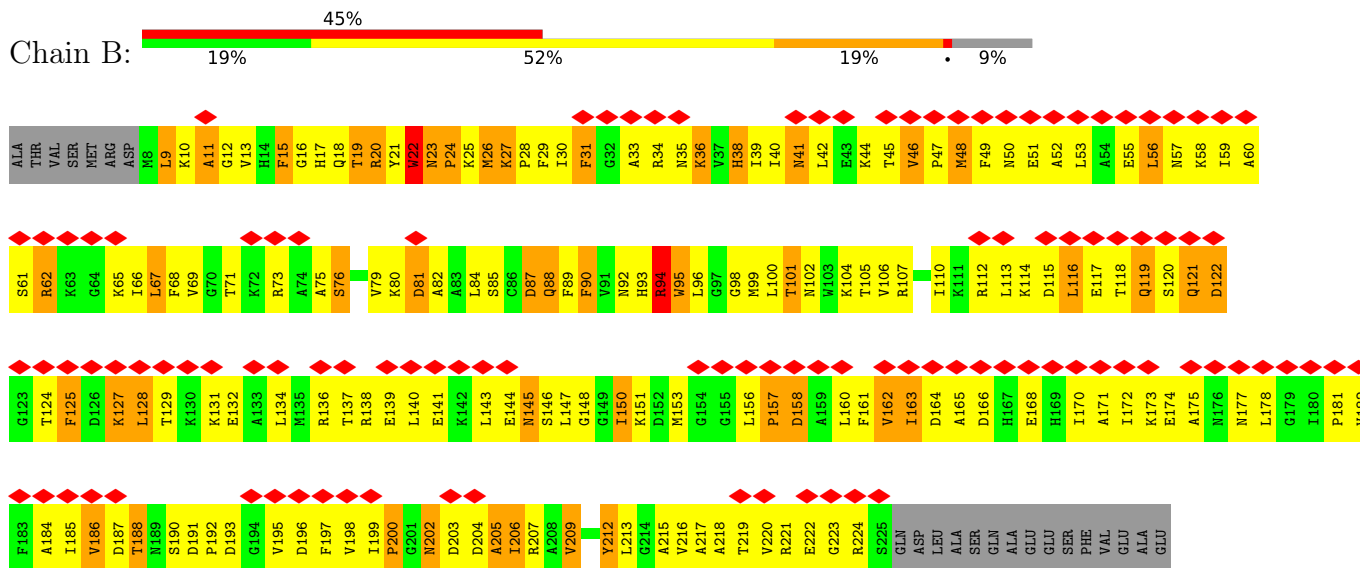




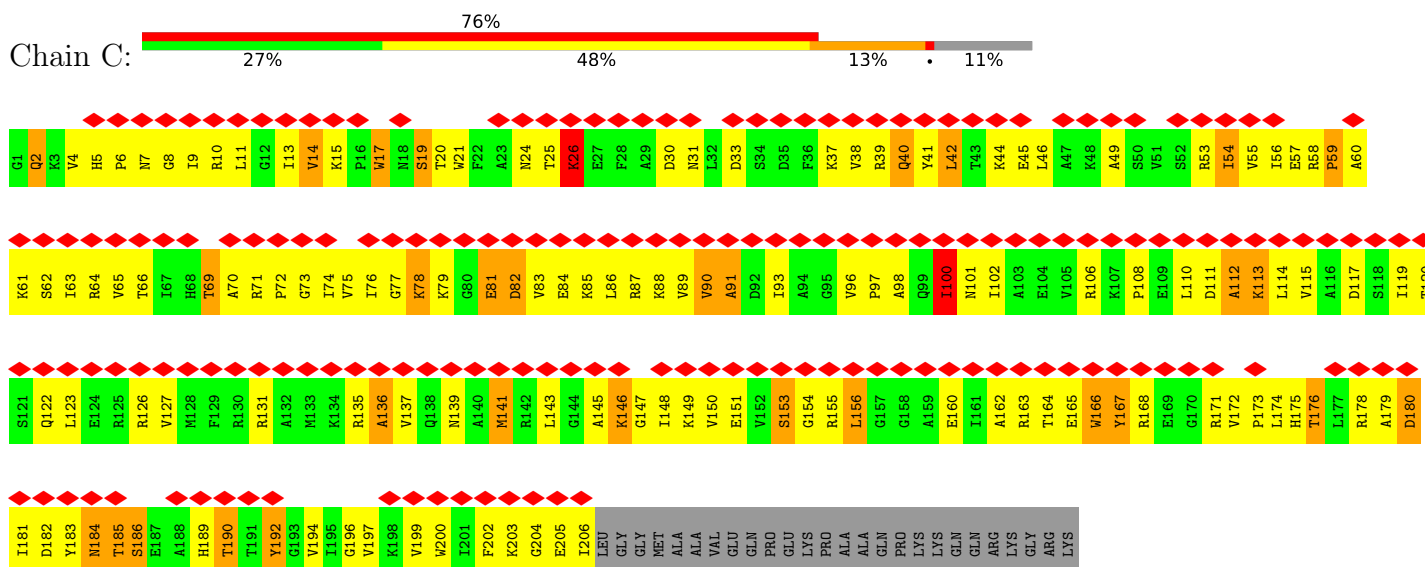




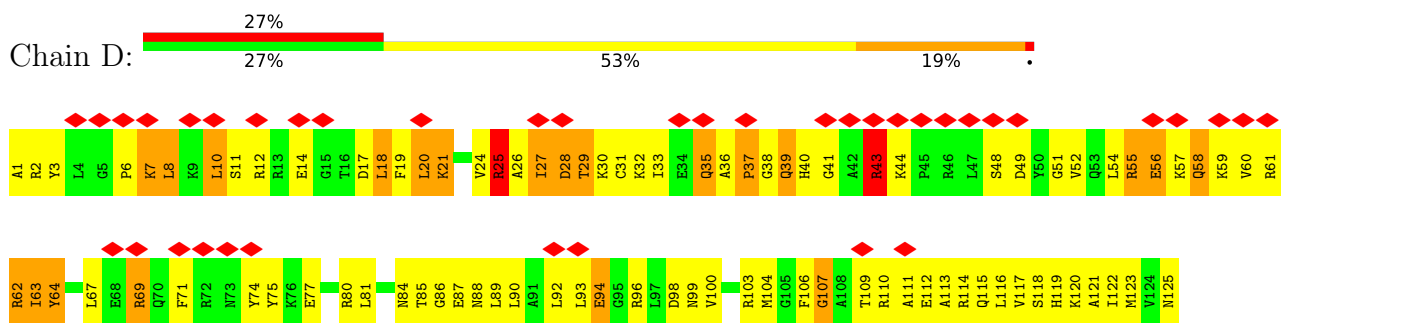
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

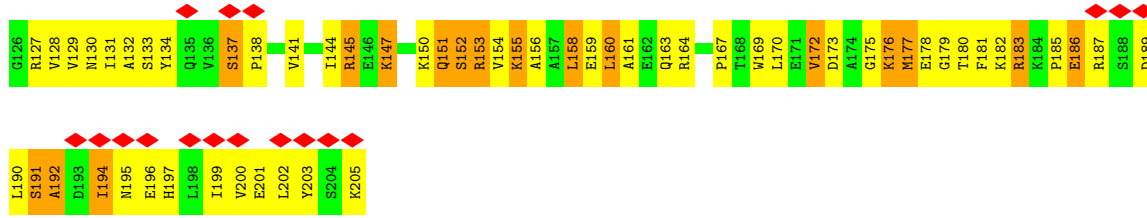


• Molecule 3: 30S RIBOSOMAL PROTEIN S3

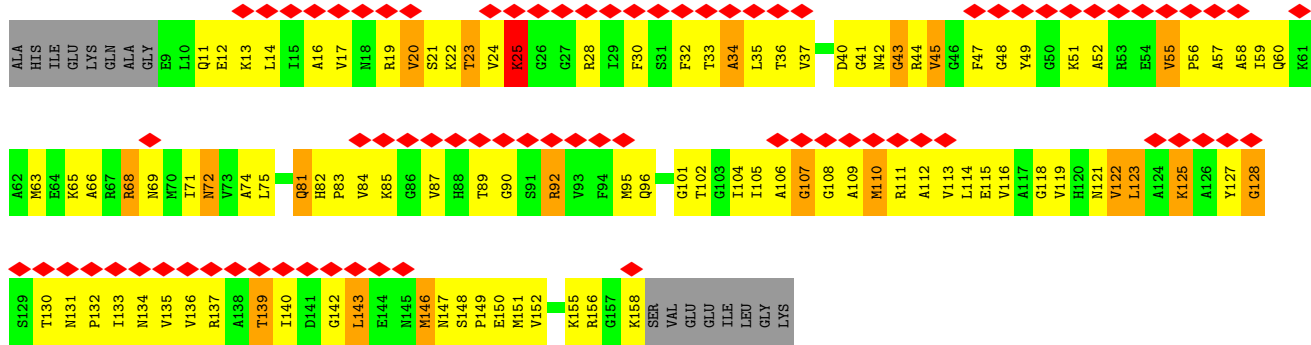


• Molecule 4: 30S RIBOSOMAL PROTEIN S4

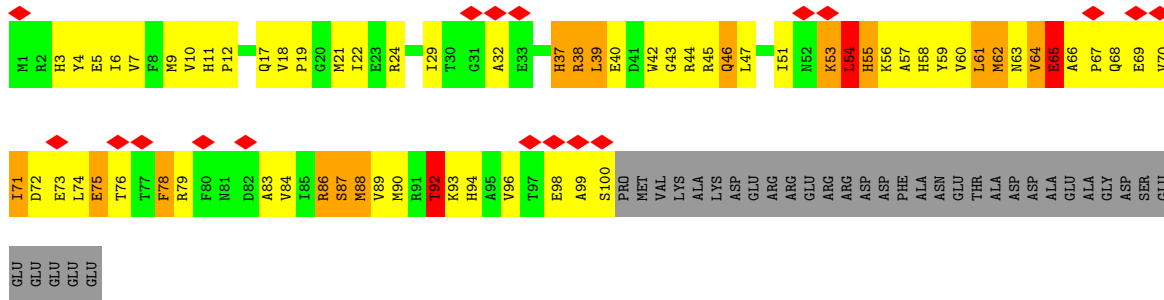
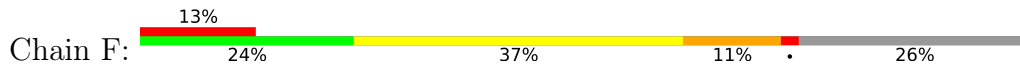




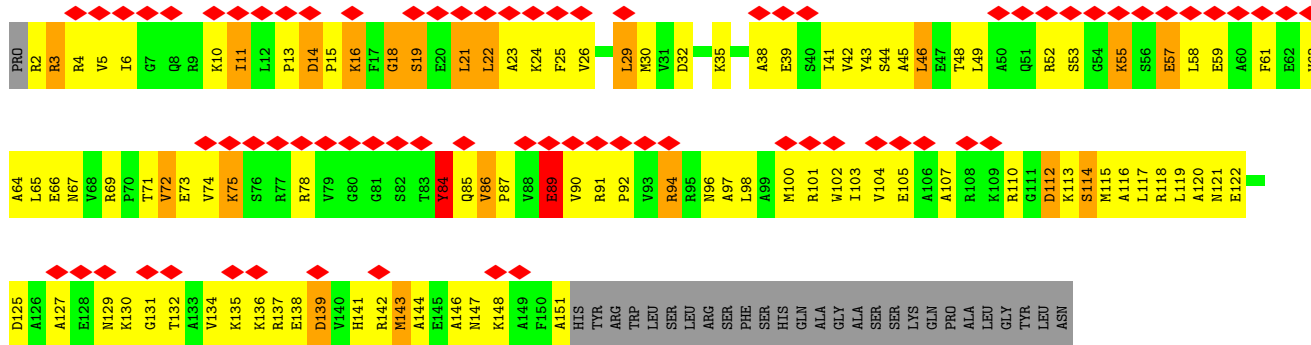
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



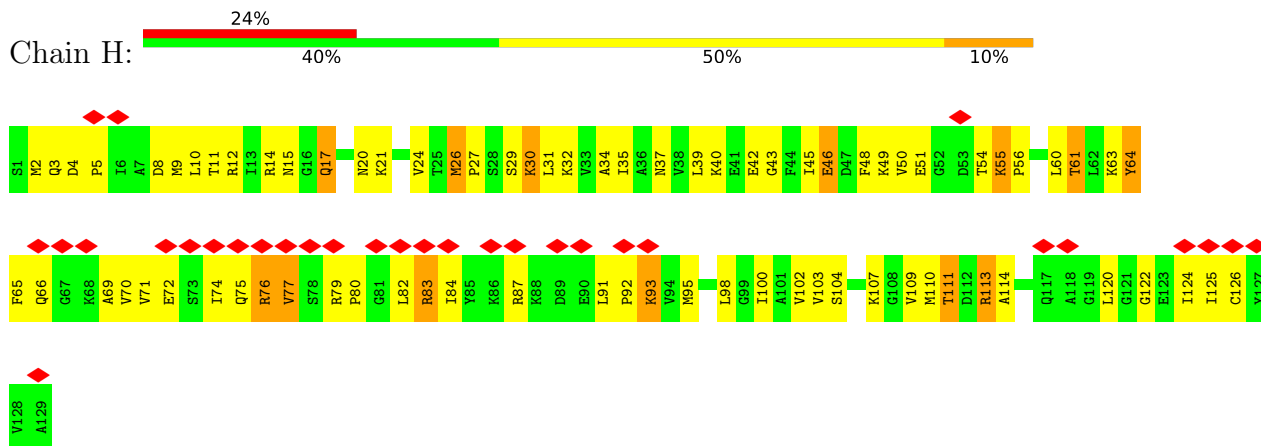
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



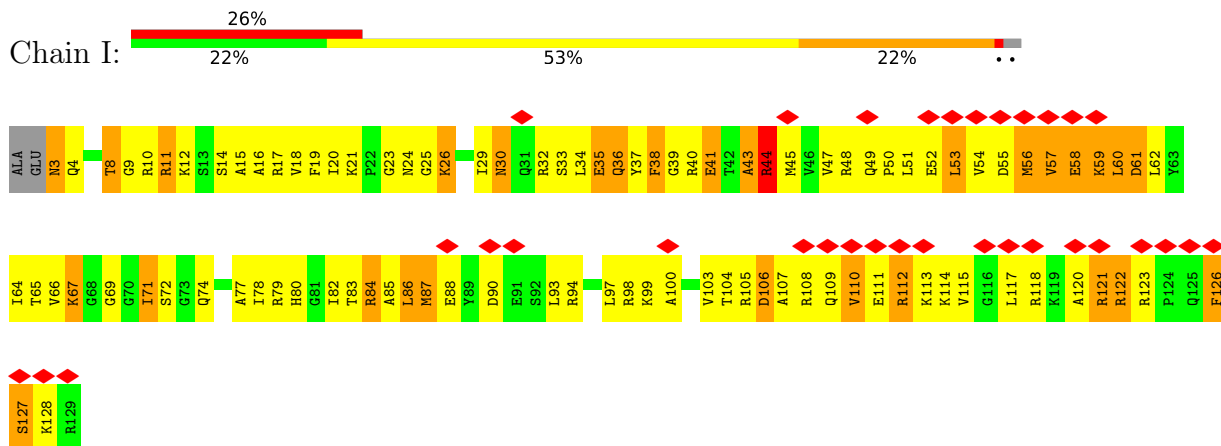
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



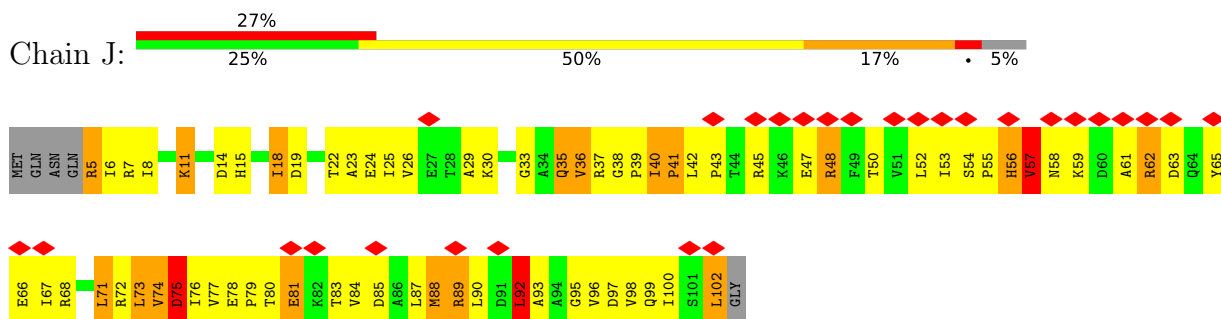
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



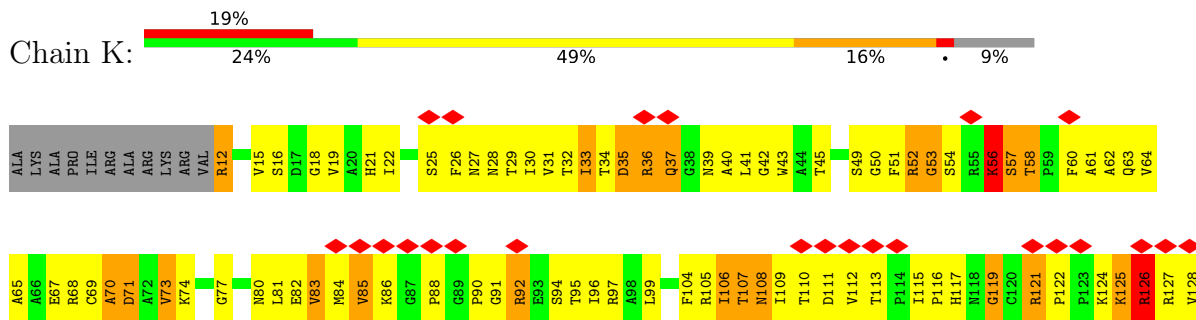
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



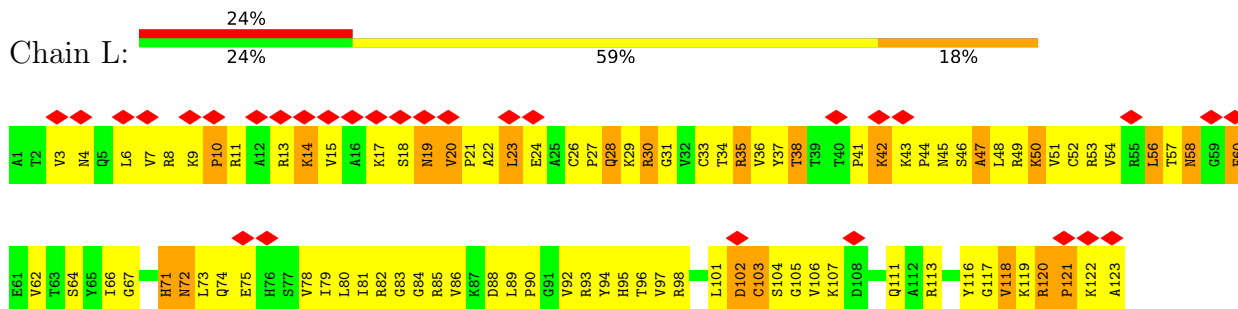
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



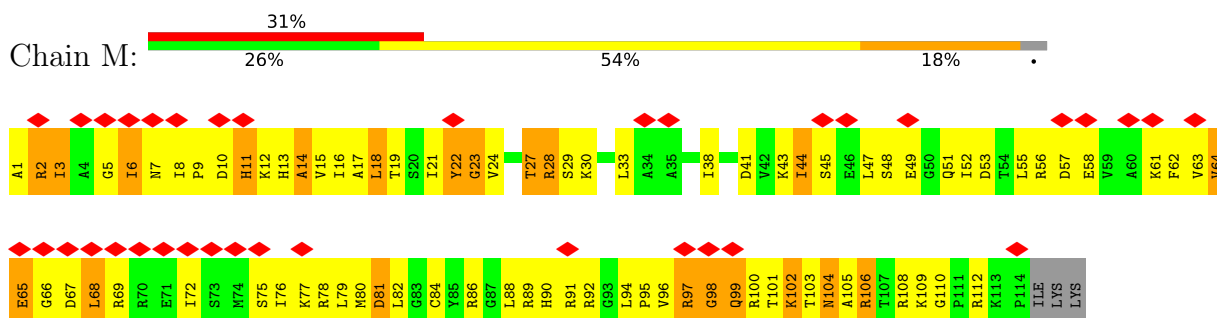
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



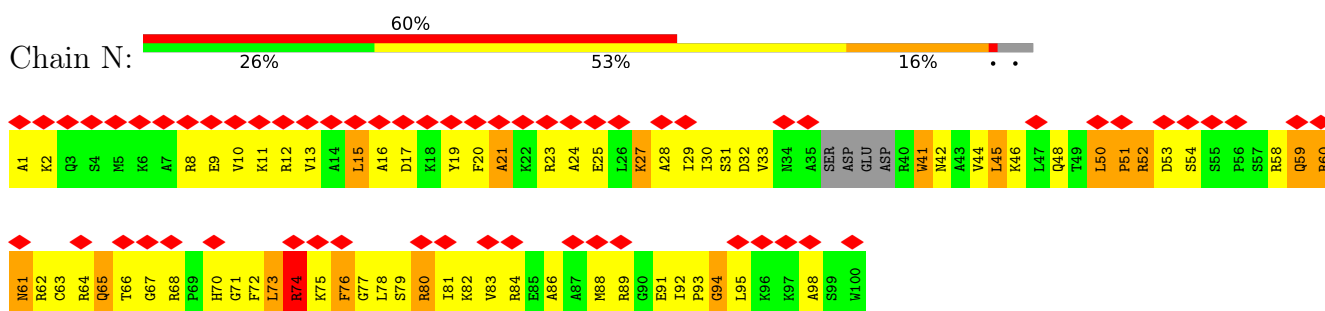
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



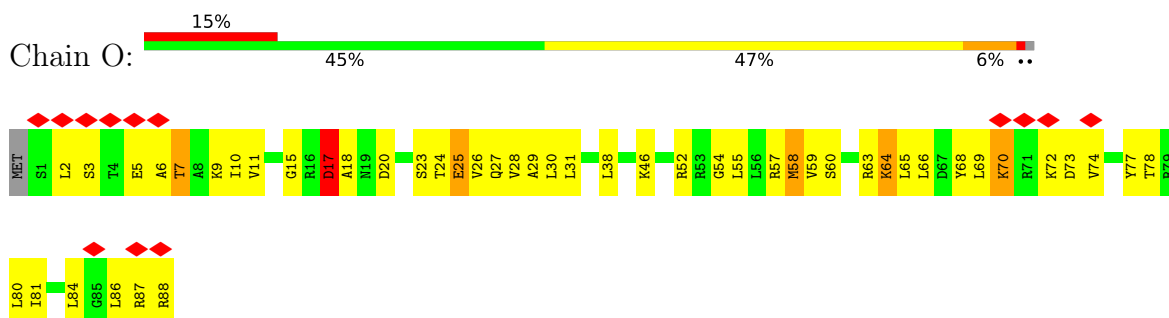
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



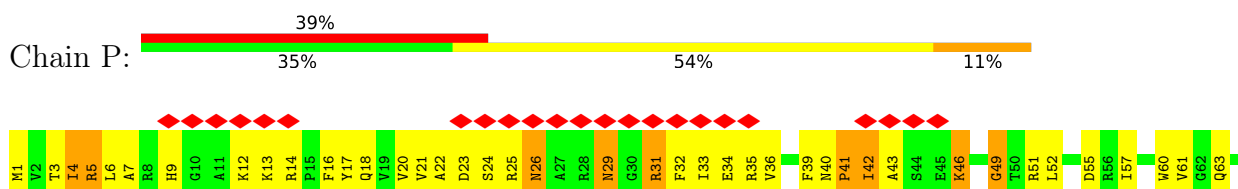
• Molecule 14: 30S RIBOSOMAL PROTEIN S14



• Molecule 15: 30S RIBOSOMAL PROTEIN S15



• Molecule 16: 30S RIBOSOMAL PROTEIN S16

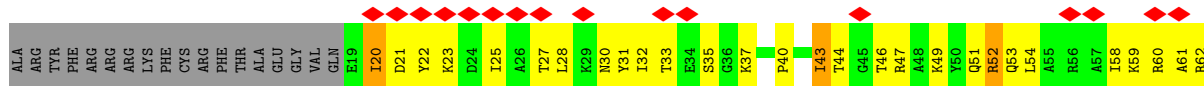
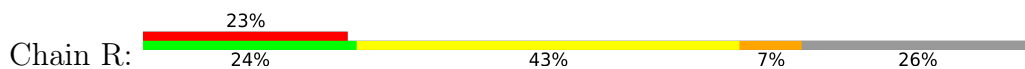




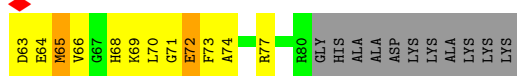
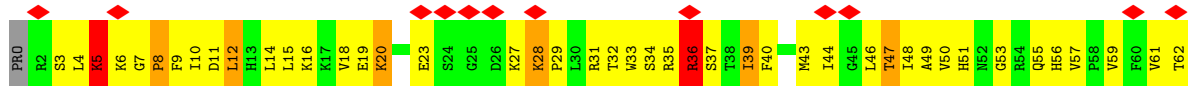
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



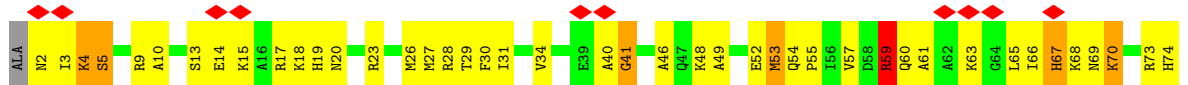
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



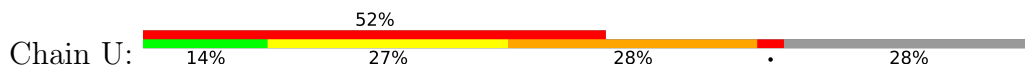
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

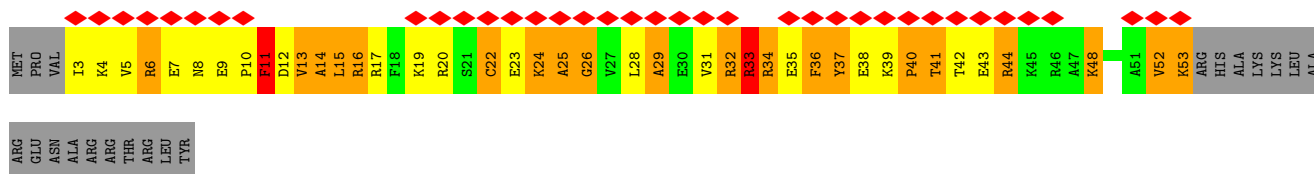


• Molecule 20: 30S RIBOSOMAL PROTEIN S20

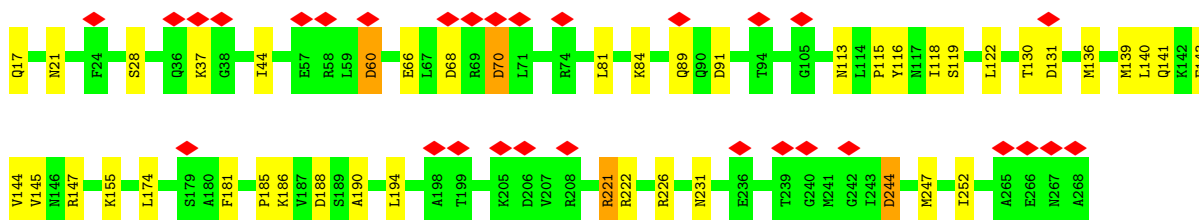
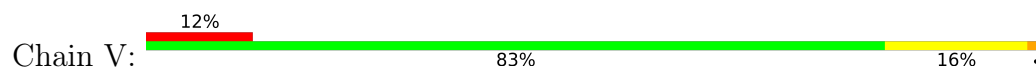


• Molecule 21: 30S RIBOSOMAL PROTEIN S21





• Molecule 22: RIBOSOMAL RNA SMALL SUBUNIT METHYLTRANSFERASE A



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	23343	Depositor
Resolution determination method	Not provided	
CTF correction method	PER IMAGE, CTFFIND3	Depositor
Microscope	FEI TECNAI 20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	82000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	615.226	Depositor
Minimum map value	-195.405	Depositor
Average map value	-10.220	Depositor
Map value standard deviation	23.595	Depositor
Recommended contour level	39.0	Depositor
Map size ( $\text{\AA}$ )	392.96, 392.96, 392.96	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	3.07, 3.07, 3.07	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.27	2/33885 (0.0%)	0.75	7/52858 (0.0%)
2	B	0.25	0/1735	0.47	0/2338
3	C	0.23	0/1651	0.45	0/2225
4	D	0.23	0/1665	0.46	0/2227
5	E	0.23	0/1118	0.45	0/1504
6	F	0.25	0/835	0.48	0/1128
7	G	0.23	0/1187	0.44	0/1591
8	H	0.23	0/989	0.45	0/1326
9	I	0.24	0/1034	0.45	0/1375
10	J	0.23	0/796	0.49	0/1077
11	K	0.24	0/893	0.46	0/1205
12	L	0.22	0/969	0.47	0/1300
13	M	0.21	0/892	0.48	0/1193
14	N	0.25	0/785	0.46	0/1043
15	O	0.23	0/724	0.45	0/966
16	P	0.26	0/659	0.44	0/884
17	Q	0.24	0/657	0.46	0/881
18	R	0.23	0/462	0.46	0/621
19	S	0.25	0/652	0.46	0/877
20	T	0.24	0/671	0.41	0/888
21	U	1.01	4/430 (0.9%)	0.74	2/570 (0.4%)
22	V	0.62	0/1991	0.80	7/2710 (0.3%)
All	All	0.29	6/54680 (0.0%)	0.68	16/80787 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	15
21	U	0	1
All	All	0	16

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	U	15	LEU	C-N	-15.01	0.99	1.34
21	U	25	ALA	C-N	-9.28	1.16	1.33
1	A	463	U	O3'-P	-6.70	1.53	1.61
21	U	29	ALA	C-N	6.63	1.49	1.34
21	U	11	PHE	C-N	-5.36	1.21	1.34

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	765	G	N9-C1'-C2'	-8.16	103.02	112.00
22	V	221	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	A	438	U	N1-C1'-C2'	-6.29	105.08	112.00
22	V	221	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	232	G	C5'-C4'-C3'	-6.21	106.07	116.00

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	G	Sidechain
1	A	281	G	Sidechain
1	A	437	U	Sidechain
1	A	438	U	Sidechain
1	A	58	C	Sidechain

## 5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	30262	0	15198	1460	0
2	B	1704	0	1720	428	0
3	C	1624	0	1699	158	0
4	D	1643	0	1710	176	0
5	E	1105	0	1145	170	0
6	F	817	0	808	76	0
7	G	1174	0	1230	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	979	0	1032	81	0
9	I	1022	0	1070	141	0
10	J	786	0	828	96	0
11	K	877	0	887	107	0
12	L	955	0	1019	103	0
13	M	883	0	944	84	0
14	N	774	0	827	92	0
15	O	716	0	742	50	0
16	P	649	0	666	78	0
17	Q	648	0	691	81	0
18	R	455	0	478	39	0
19	S	637	0	665	78	0
20	T	665	0	714	53	0
21	U	425	0	447	102	0
22	V	1949	0	1949	46	0
23	V	139	0	0	11	0
All	All	50888	0	36469	3247	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 37.

The worst 5 of 3247 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:U:C6	2:B:27:LYS:HD3	1.28	1.64
1:A:829:G:C3'	2:B:30:ILE:HG12	1.18	1.62
1:A:830:G:C4	2:B:22:TRP:HB3	1.40	1.53
1:A:17:U:C5'	1:A:1079:G:H5'	1.39	1.49
1:A:830:G:C5	2:B:22:TRP:HB3	1.47	1.49

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	216/240 (90%)	145 (67%)	53 (24%)	18 (8%)	1	12
3	C	204/232 (88%)	135 (66%)	49 (24%)	20 (10%)	0	10
4	D	203/205 (99%)	130 (64%)	55 (27%)	18 (9%)	1	11
5	E	148/166 (89%)	108 (73%)	33 (22%)	7 (5%)	2	21
6	F	98/135 (73%)	69 (70%)	23 (24%)	6 (6%)	1	17
7	G	148/178 (83%)	103 (70%)	37 (25%)	8 (5%)	2	19
8	H	127/129 (98%)	105 (83%)	19 (15%)	3 (2%)	6	33
9	I	125/129 (97%)	86 (69%)	28 (22%)	11 (9%)	1	11
10	J	96/103 (93%)	63 (66%)	21 (22%)	12 (12%)	0	5
11	K	115/128 (90%)	75 (65%)	27 (24%)	13 (11%)	0	7
12	L	121/123 (98%)	74 (61%)	30 (25%)	17 (14%)	0	4
13	M	112/117 (96%)	87 (78%)	14 (12%)	11 (10%)	0	10
14	N	92/100 (92%)	59 (64%)	24 (26%)	9 (10%)	0	10
15	O	86/89 (97%)	66 (77%)	18 (21%)	2 (2%)	6	34
16	P	80/82 (98%)	59 (74%)	17 (21%)	4 (5%)	2	20
17	Q	78/83 (94%)	48 (62%)	26 (33%)	4 (5%)	2	19
18	R	53/74 (72%)	27 (51%)	19 (36%)	7 (13%)	0	5
19	S	77/91 (85%)	57 (74%)	14 (18%)	6 (8%)	1	13
20	T	83/86 (96%)	69 (83%)	8 (10%)	6 (7%)	1	14
21	U	49/71 (69%)	22 (45%)	12 (24%)	15 (31%)	0	0
22	V	250/252 (99%)	247 (99%)	2 (1%)	1 (0%)	34	72
All	All	2561/2813 (91%)	1834 (72%)	529 (21%)	198 (8%)	2	13

5 of 198 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	19	THR
2	B	22	TRP
2	B	163	ILE
2	B	186	VAL
3	C	2	GLN

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	180/198 (91%)	142 (79%)	38 (21%)	1	6
3	C	170/189 (90%)	142 (84%)	28 (16%)	2	12
4	D	172/172 (100%)	140 (81%)	32 (19%)	1	9
5	E	113/125 (90%)	92 (81%)	21 (19%)	1	9
6	F	87/116 (75%)	68 (78%)	19 (22%)	1	6
7	G	123/146 (84%)	102 (83%)	21 (17%)	2	11
8	H	104/104 (100%)	87 (84%)	17 (16%)	2	13
9	I	105/106 (99%)	83 (79%)	22 (21%)	1	6
10	J	86/90 (96%)	66 (77%)	20 (23%)	1	4
11	K	90/98 (92%)	70 (78%)	20 (22%)	1	6
12	L	103/103 (100%)	88 (85%)	15 (15%)	3	15
13	M	92/95 (97%)	70 (76%)	22 (24%)	0	4
14	N	79/83 (95%)	67 (85%)	12 (15%)	3	14
15	O	76/77 (99%)	69 (91%)	7 (9%)	9	29
16	P	65/65 (100%)	56 (86%)	9 (14%)	3	17
17	Q	74/77 (96%)	60 (81%)	14 (19%)	1	8
18	R	48/64 (75%)	45 (94%)	3 (6%)	18	43
19	S	70/78 (90%)	60 (86%)	10 (14%)	3	16
20	T	65/65 (100%)	56 (86%)	9 (14%)	3	17
21	U	44/61 (72%)	36 (82%)	8 (18%)	1	10
22	V	213/216 (99%)	206 (97%)	7 (3%)	38	61
All	All	2159/2328 (93%)	1805 (84%)	354 (16%)	5	12

5 of 354 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	92	ARG
14	N	76	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
12	L	18	SER
13	M	44	ILE
16	P	46	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
15	O	39	GLN
16	P	18	GLN
20	T	12	GLN
5	E	134	ASN
5	E	131	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1407/1542 (91%)	261 (18%)	24 (1%)

5 of 261 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	A
1	A	9	G
1	A	14	U
1	A	31	G
1	A	32	A

5 of 24 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1025	U
1	A	1101	A
1	A	1065	U
1	A	1181	G
1	A	372	C

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
21	U	2
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	929:G	O3'	930:C	P	7.59
1	U	25:ALA	C	26:GLY	N	1.16
1	U	15:LEU	C	16:ARG	N	0.99

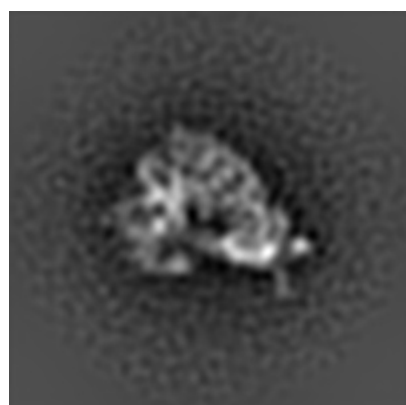
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2017. These allow visual inspection of the internal detail of the map and identification of artifacts.

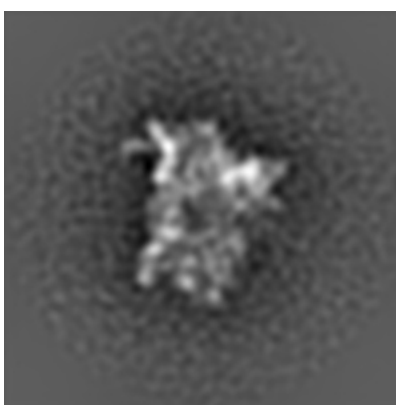
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

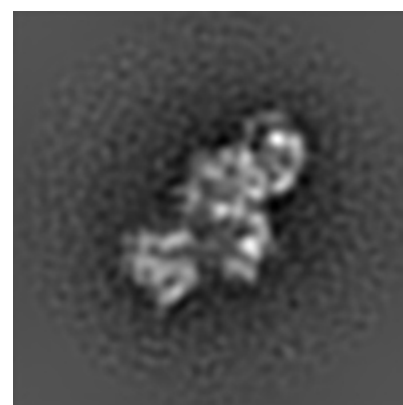
#### 6.1.1 Primary map



X



Y

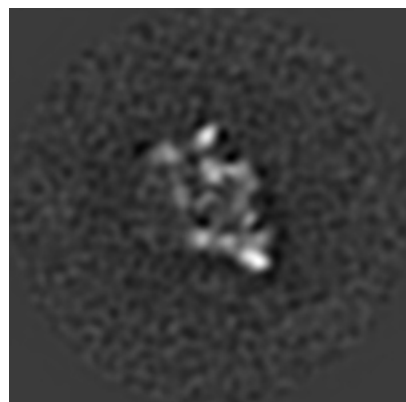


Z

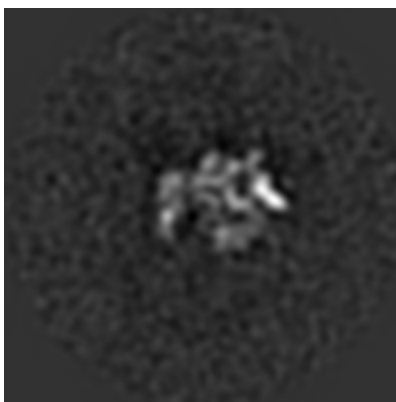
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

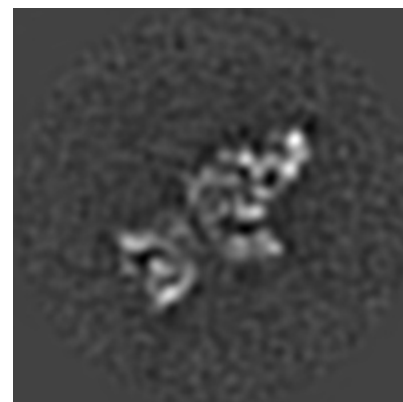
#### 6.2.1 Primary map



X Index: 64



Y Index: 64



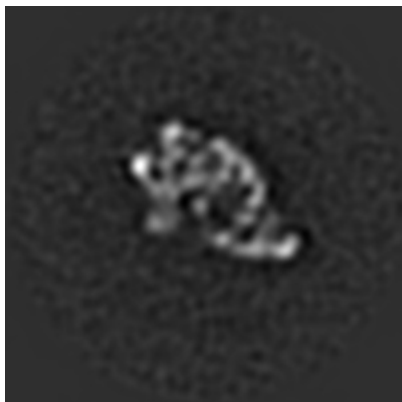
Z Index: 64



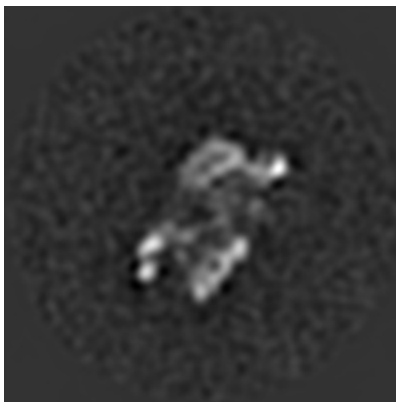
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

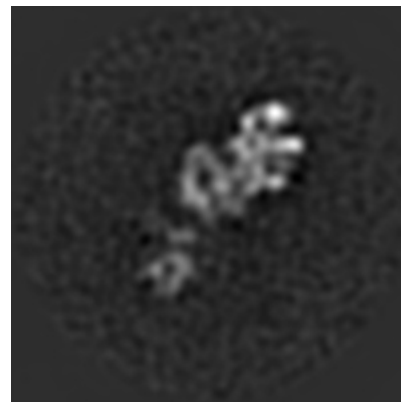
### 6.3.1 Primary map



X Index: 75



Y Index: 53

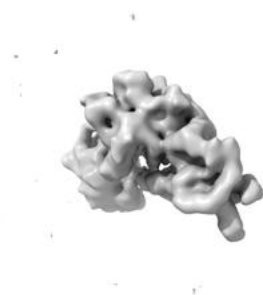


Z Index: 51

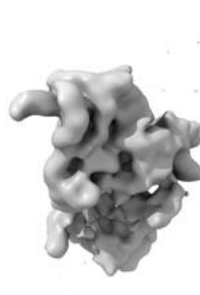
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 39.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

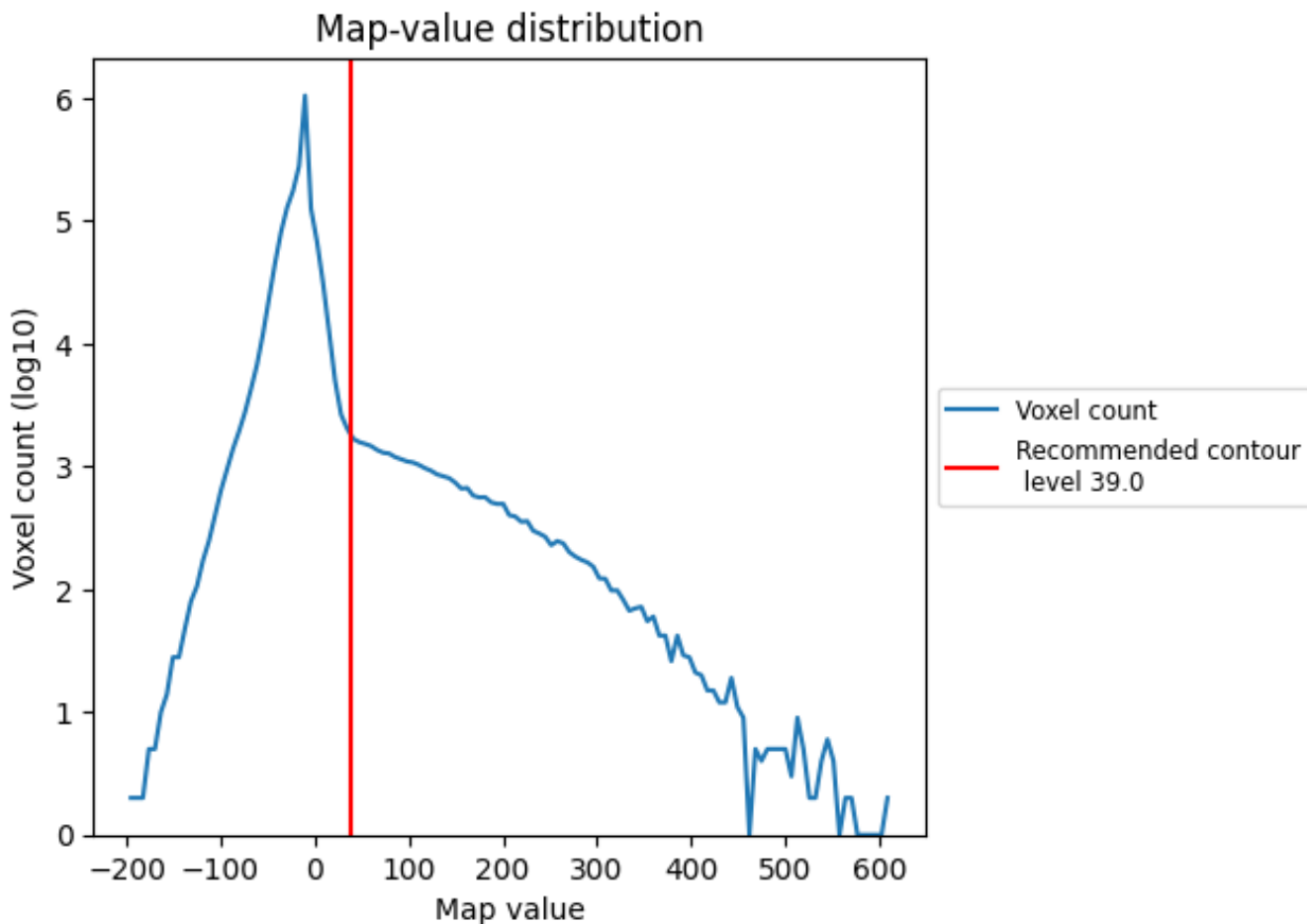
## 6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

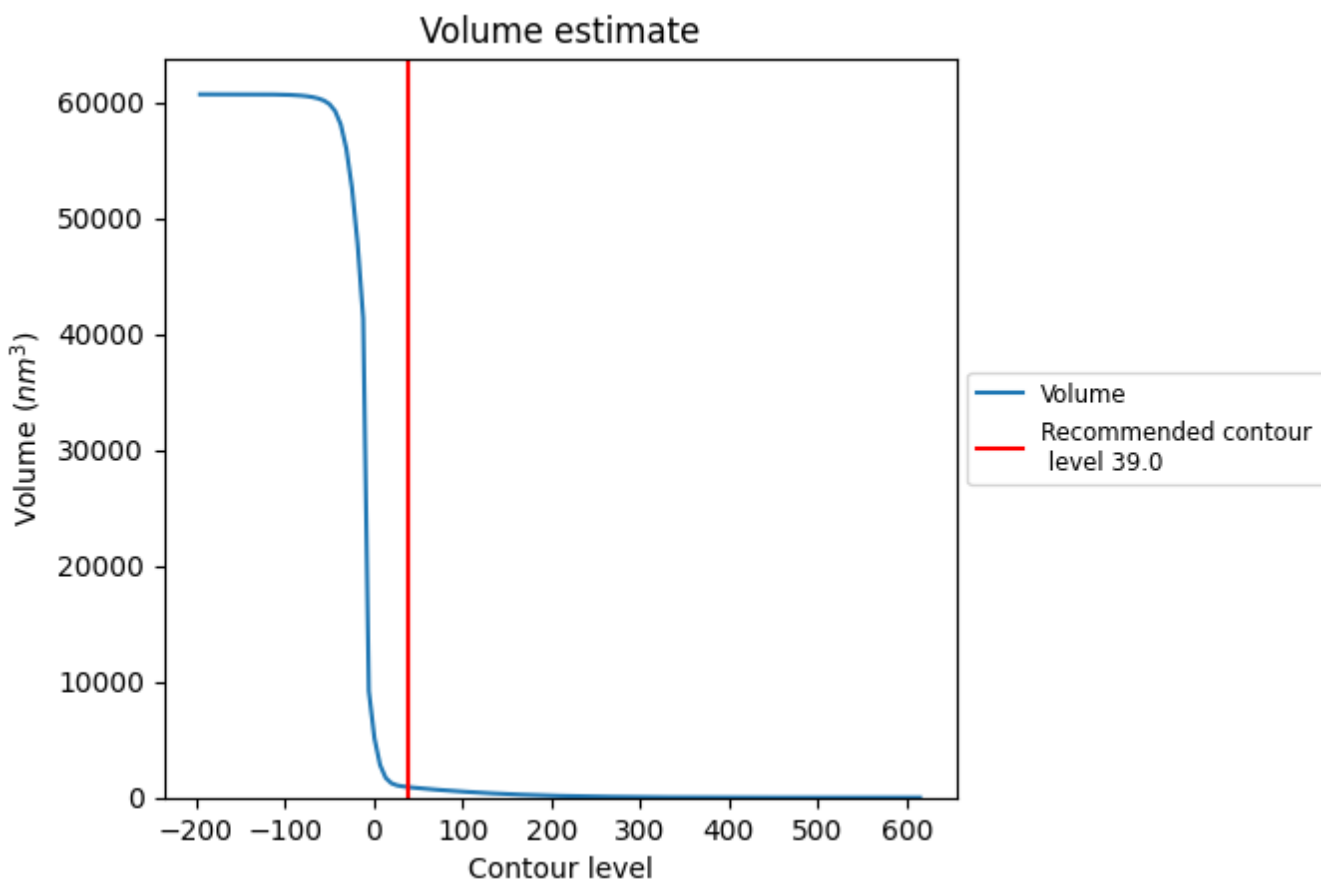
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

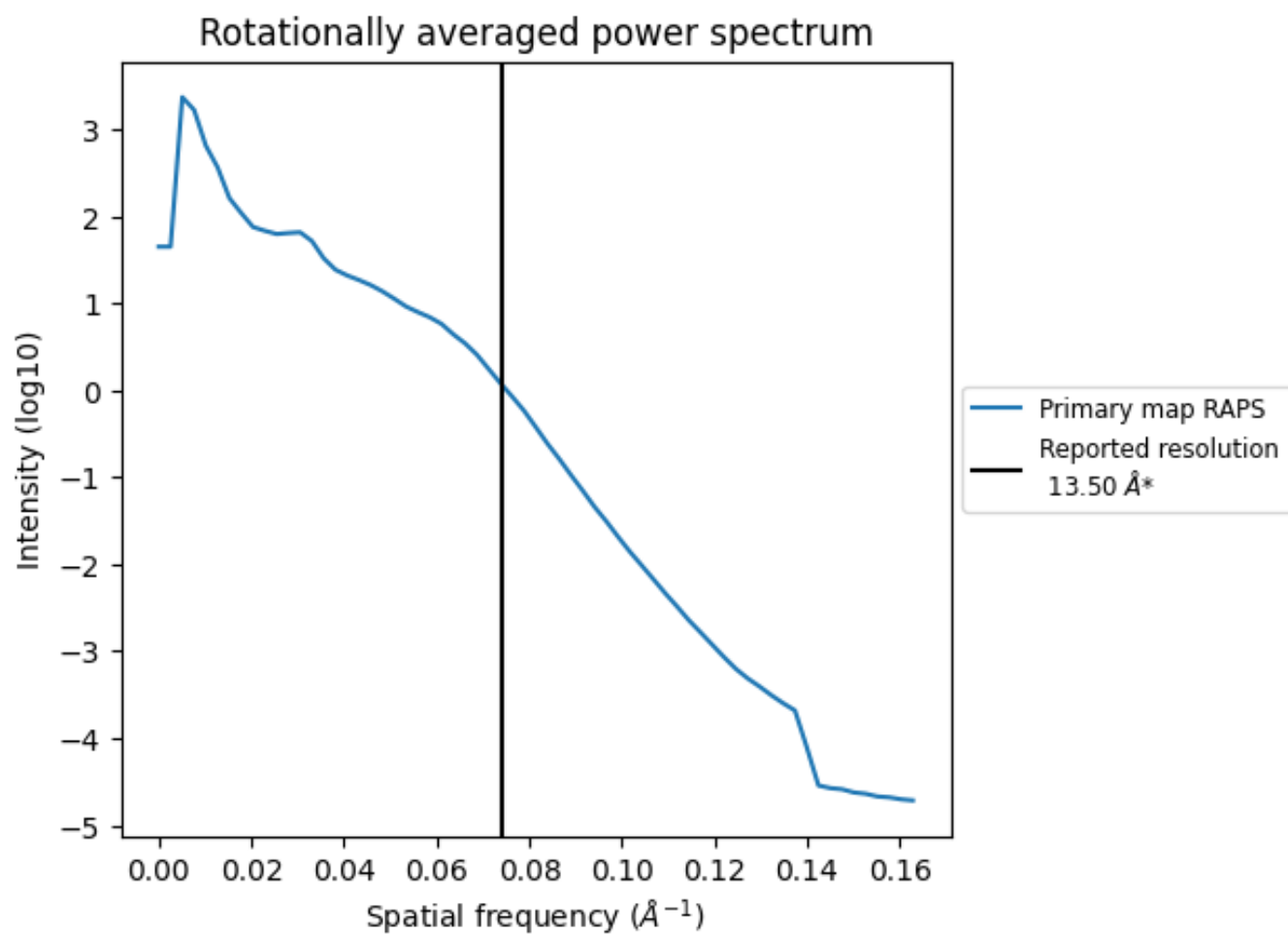
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 902 nm<sup>3</sup>; this corresponds to an approximate mass of 815 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of 0.074 Å<sup>-1</sup>

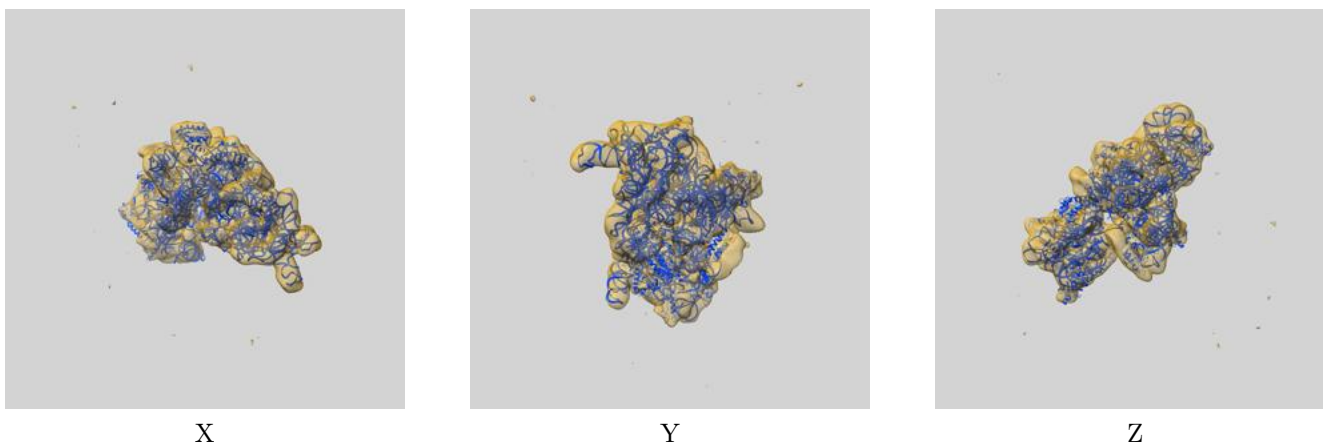
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

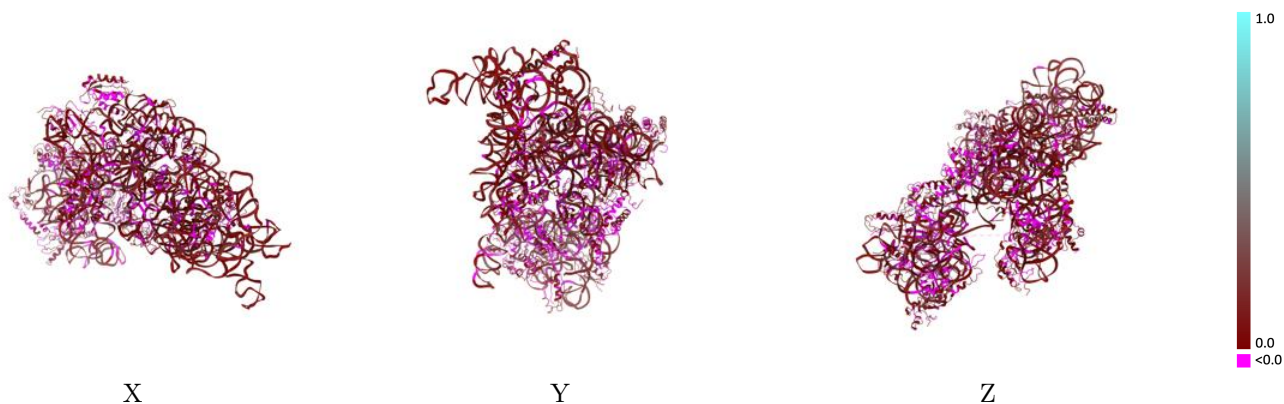
This section contains information regarding the fit between EMDB map EMD-2017 and PDB model 4ADV. Per-residue inclusion information can be found in section 3 on page 8.

### 9.1 Map-model overlay [i](#)



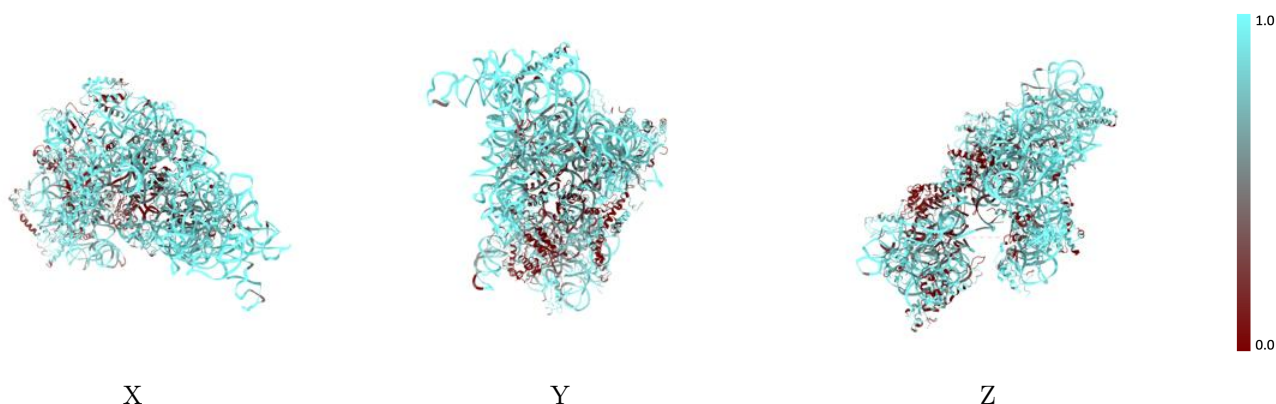
The images above show the 3D surface view of the map at the recommended contour level 39.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

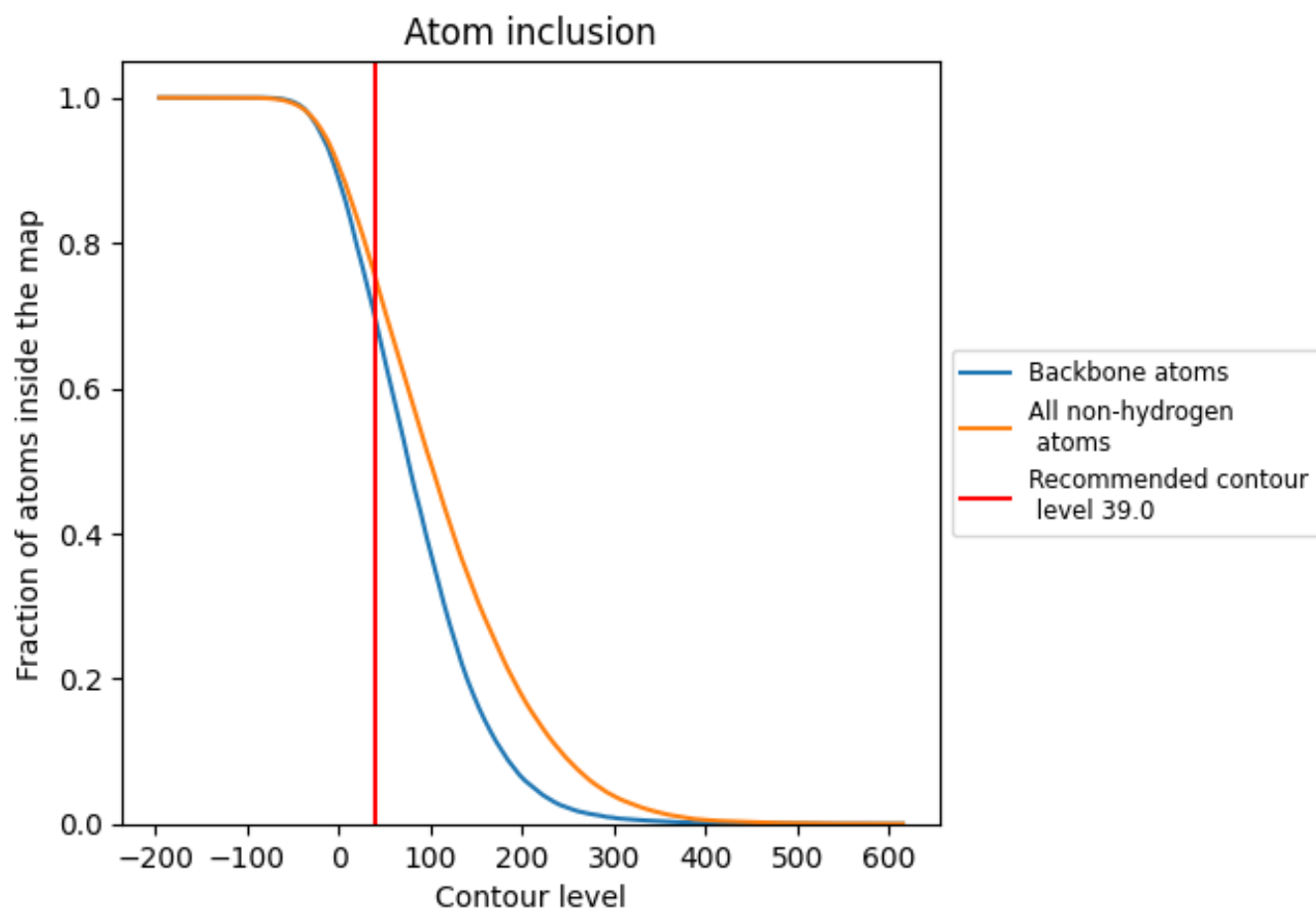
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (39.0).

















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (39.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7570	 0.0610
A	 0.8594	 0.0810
B	 0.4824	 0.0100
C	 0.1217	 0.0090
D	 0.6610	 0.0230
E	 0.4718	 0.0700
F	 0.7613	 0.0440
G	 0.4547	 0.0460
H	 0.7323	 0.0370
I	 0.6691	 0.0260
J	 0.6557	 0.0130
K	 0.7175	 0.0360
L	 0.6895	 0.0310
M	 0.6287	 0.0300
N	 0.3324	 -0.0020
O	 0.8217	 0.0540
P	 0.5885	 0.0130
Q	 0.6899	 0.0790
R	 0.6743	 0.0040
S	 0.8213	 0.0420
T	 0.8108	 0.0440
U	 0.2562	 0.0160
V	 0.8288	 0.0480

